The Canadian Mineralogist
Vol. 50, pp. 45-53 (2012)
DOI: 10.3749/canmin.50.1.45

POSTITE, $Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})\bullet 13H_2O$, A NEW MINERAL SPECIES FROM THE LA SAL MINING DISTRICT, UTAH: CRYSTAL STRUCTURE AND DESCRIPTIVE MINERALOGY

ANTHONY R. KAMPF[§]

Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, U.S.A.

JOHN M. HUGHES

Department of Geology, The University of Vermont, Burlington, Vermont 05405, U.S.A.

JOE MARTY

5199 E. Silver Oak Rd., Salt Lake City, Utah 84108, U.S.A.

BARBARA NASH

Department of Geology and Geophysics, University of Utah, Salt Lake City, Utah 84112, U.S.A.

ABSTRACT

Postite, $Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})\bullet 13H_2O$, is a new mineral species from the Vanadium Queen mine, La Sal Creek Canyon, and the Blue Cap mine, Lyon Canyon Creek, San Juan County, Utah, U.S.A. Postite occurs as very thin, needle-like prisms with pyramidal terminations; crystals commonly occur in parallel bundles and grow in divergent and "jackstraw" masses. Individual crystals are up to 1 mm long and 50 μm in diameter, and are golden-yellow with a yellow streak. The mineral is transparent, with a subadamantine luster; it does not fluoresce in short- or long-wave ultraviolet radiation. Postite has a Mohs hardness of approximately 2 and brittle tenacity. The mineral has one good cleavage on {001} and at least two perfect cleavages parallel to [001], possibly {100} and {010}. The fracture is splintery. The density calculated from the empirical formula using the single-crystal cell data is 2.226 g/cm^3. Postite is biaxial (+) with a 2*V* angle of 71°. Indices of refraction for postite are α 1.727(3), β 1.733(3), and γ 1.745(3). The optical orientation is X = **c**, Y = **b**, Z = **a**. Dispersion was not observed and pleochroism was not perceptible. Electron probe microanalysis and the crystal structure solution gave the empirical formula $(Mg_{0.97}Na_{0.06}Ca_{0.04}Sr_{0.01}K_{0.01})_{\Sigma 1.09}Al_{1.94}[(OH)_{1.92}(H_2O)_{0.08}]_{\Sigma 2.00}(V_{10}O_{28})\bullet 27H_2O$. The simplified structural formula of postite is $Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})\bullet 13H_2O$. Postite is orthorhombic, *Pccn*, with *a* 16.3357(6), *b* 24.2434(17), *c* 11.7343(4) Å, *V* 4647.2(4) Å^3, and $Z = 4$. The strongest four lines in the diffraction pattern are [*d* in Å(I)(*hkl*)]: 8.937(100)(111), 12.190(90)(020), 3.771(24)(113), and 8.248(22)(200). The atomic arrangement of postite was solved and refined to $R_1 = 0.0358$. The structural unit is a decavanadate polyanion, $[V_{10}O_{28}]^{6-}$; charge balance in the structure is maintained by the $[Mg(H_2O)_6Al_2(OH)_2(H_2O)_8\bullet 13H_2O]^{6+}$ interstitial unit. The interstitial unit consists of a $[Mg(H_2O)_6]^{2+}$ monomer, an $[Al_2(OH)_2(H_2O)_8]^{4+}$ edge-sharing dimer, and thirteen additional H_2O molecules. The linkage between the structural unit and the interstitial unit results from hydrogen bonding between oxygen atoms of the structural unit with hydrogen atoms of the $[Al_2(OH)_2(H_2O)_8]^{4+}$ edge-sharing dimer and those of isolated H_2O molecules. The new mineral is named in honor of Dr. Jeffrey E. Post (b. 1954), Curator-in-Charge of the National Gem and Mineral Collection, U. S. National Museum of Natural History (Smithsonian Institution).

Keywords: postite, new mineral species, decavanadate, crystal structure, Vanadium Queen Mine, La Sal district, Utah

§ *E-mail address:* akampf@nhm.org

Introduction

The uranium and vanadium (*Uravan*) deposits of Colorado and Utah have been a rich source of ore in the production of these metals. Uranium and vanadium minerals in the La Sal area, Utah, as elsewhere in the Colorado Plateau Uravan mineral belt, occur together as bedded or roll-front deposits, impregnating sandstone of the Salt Wash member of the Jurassic Morrison Formation (Carter & Gualtieri 1965, Shawe 2011). In these deposits, a variety of unusual secondary vanadium minerals form from the oxidation of vanadium orebodies at low temperatures. Collecting by one of the authors (JM) at several Colorado Plateau Uravan deposits in Colorado and Utah has led to the discovery of many new species. Except for martyite, $Zn_3(V_2O_7)(OH)_2 \bullet 2H_2O$ (Kampf & Steele 2008b), which contains the divanadate group $[V_2O_7]^{4-}$, and dickthomssenite, $Mg(V_2O_6) \bullet 7H_2O$ (Hughes *et al.* 2001), which contains $[VO_3]^-$ vanadate chains, all of the new species contain the decavanadate anionic complex $[V_{10}O_{28}]^{6-}$ and are members of the pascoite, $Ca_3[V_{10}O_{28}] \bullet 17H_2O$ (Hughes *et al.* 2005), family of minerals. The new decavanadates include gunterite, $Na_4(H_2O)_{16}(H_2V_{10}O_{28}) \bullet 6H_2O$ (Kampf *et al.* 2011b), hughesite, $Na_3Al(V_{10}O_{28}) \bullet 22H_2O$ (Rakovan *et al.* 2011), lasalite, $Na_2Mg_2[V_{10}O_{28}] \bullet 20H_2O$ (Hughes *et al.* 2008), magnesiopascoite, $Ca_2Mg[V_{10}O_{28}] \bullet 16H_2O$ (Kampf & Steele 2008a), and rakovanite, $Na_3\{H_3[V_{10}O_{28}]\} \bullet 15H_2O$ (Kampf *et al.* 2011a). The collecting also yielded crystals of the decavanadate huemulite, $Na_4Mg[V_{10}O_{28}] \bullet 24H_2O$ (Gordillo *et al.* 1966), suitable for structure determination (Colombo *et al.* 2011). The only other previously known mineral of the pascoite family, hummerite, $K_2Mg_2[V_{10}O_{28}] \bullet 16H_2O$ (Hughes *et al.* 2002), also comes from the Uravan deposits.

Herein, we describe another new member of the pascoite family from the Uravan deposits. The new mineral species was discovered at the Vanadium Queen mine and subsequently was found in the same stratigraphic horizon at the nearby Blue Cap mine. The new mineral is named postite in honor of Dr. Jeffrey E. Post (b. 1954), Curator-in-Charge of the National Gem and Mineral Collection, U. S. National Museum of Natural History (Smithsonian Institution). Dr. Post has had a long and distinguished career in mineralogy, crystallography, and geochemistry and has made important contributions to the scientific understanding of manganese oxide minerals, in particular. The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2011-060). The two cotype specimens used in the description of the mineral are housed in the mineral collection of the Natural History Museum of Los Angeles County under catalogue numbers 63564 (Vanadium Queen mine) and 63563 (Blue Cap mine).

Occurrence

Postite was first found on sandstone blocks in the Vanadium Queen mine (38°20'11"N, 109°04'58"W), 18 km east of La Sal, San Juan County, Utah, U.S.A. Subsequently, better crystals of postite were found at the Blue Cap mine (38°21'14"N, 109°03'39"W), Lyon Canyon Creek, which is in the same stratigraphic horizon, east of the first location.

The new mineral species is rare. Crystals are found growing as needles on corvusite-montroseite-bearing sandstone blocks. Other minerals found nearby include barite, calcite, clausthalite, devilline, dickthomssenite, hewettite, lasalite, magnesiopascoite, martyite, natrozippeite, navajoite, paramontroseite, pascoite, pyrite, rossite, selenium, sherwoodite, sulfur, tyuyamunite, uranopilite, and zeunerite.

The mineral forms from the oxidation of montroseite-corvusite assemblages in a moist environment. Mining operations have exposed unoxidized and oxidized phases. Under ambient temperatures and generally oxidizing near-surface environments, water reacts with pyrite in the deposit to form aqueous solutions with a relatively low pH. The various secondary vanadate phases that formed depend upon the Eh-pH and presence of other cations (*e.g.*, Na^+, Ca^{2+}, Mg^{2+}, Al^{3+}) (*e.g.*, Evans & Garrels 1958).

Appearance and Physical Properties

Crystals of postite are very thin, needle-like prisms with pyramidal terminations; some needles are slightly curved (Fig. 1). Crystals generally occur in parallel bundles and grow in divergent and "jackstraw" masses. Individual crystals are up to 1 mm long and 50 μm in diameter (Fig. 2).

Postite is golden yellow in color and has a yellow streak. The mineral is transparent and exhibits a subadamantine luster. It does not fluoresce in short- or long-wave ultraviolet radiation. Postite has a Mohs hardness of approximately 2 and a brittle tenacity. The mineral has one good cleavage on {001} and at least two perfect cleavages parallel to [001], possibly on {100} and {010}; no parting was observed. The fracture is splintery because of the cleavages parallel to [001].

The density of postite could not be measured because the mineral dissolves in an aqueous sodium polytungstate solution, and there is insufficient material for direct measurement. The calculated density is 2.226 g cm^{-3}, based on the empirical formula and using single-crystal cell data. On the basis of the ideal formula, the calculated density is 2.224 g/cm^3. Postite was not observed to dissolve in distilled water but dissolves rapidly in dilute HCl.

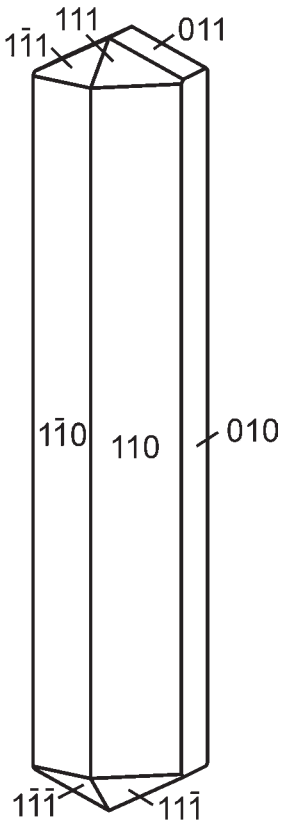

FIG 1. Crystal drawing (clinographic projection) of postite obtained on the basis of reflecting goniometer measurements.

OPTICAL PROPERTIES

Postite is biaxial (+) with indices of refraction α 1.727(3), β 1.733(3), and γ 1.745(3). Because of the thinness of the needles, conoscopic observations were not possible. The calculated 2*V* is 71°. Dispersion was not observed and pleochroism was not perceptible. The optical orientation is *X* = **c**, *Y* = **b**, *Z* = **a**.

THE COMPOSITION OF POSTITE

Analyses (ten from eight crystals) were performed at the University of Utah with a Cameca SX-50 electron microprobe with four wavelength-dispersive spectrometers. Analytical conditions were 15 keV accelerating voltage, 10 nA beam current and a nominal beam diameter of 10 μm, although a diameter of 15 μm was occasionally used for larger fragments. Counting times were 10 seconds for each element. Raw X-ray intensities were corrected for matrix effects with a $\varphi(\rho z)$ algorithm (Pouchou & Pichoir 1991).

Such phases as postite, gunterite, hughesite, rakovanite, and lasalite dehydrate rapidly under vacuum and the electron beam. Thus, the concentration of the remaining constituents increases with the loss of H_2O, yielding cation totals higher than expected in the fully hydrated phase. However, the stoichiometric ratios of the cations remains identical, thus the efficacy of the analysis is viewed through the stoichiometric ratio of the cations. In the absence of a direct H_2O determination, for which sufficient material is seldom available, the amount of H_2O in the sample is effectively established through the crystal structure analysis.

The average of ten analyses obtained from partially dehydrated postite is reported in column 2 of Table 1.

TABLE 1. ANALYTICAL RESULTS FOR POSTITE

Constituent	wt.%*	St. dev.	Normalized wt.%	Ideal wt.%	Probe standard
Na_2O	0.15	0.16	0.12	---	albite
K_2O	0.03	0.02	0.02	---	sanidine
MgO	3.04	0.12	2.50	2.59	diopside
CaO	0.16	0.02	0.13	---	diopside
SrO	0.10	0.08	0.08	---	celestine
Al_2O_3	7.71	0.29	6.34	6.55	sanidine
V_2O_5	71.00	1.20	58.37	58.44	V metal
H_2O	17.81		32.43§	32.42	
Total	100.00		99.99†	100.00	

* Average of 10 analyses from eight crystals of partially dehydrated postite. H_2O by difference.
§ Based upon crystal structure with O = 57
† Rounding error
The empirical formula (based on V = 10 with H_2O assigned from the structure analysis for which O = 57) is: $(Mg_{0.97}Na_{0.06}Ca_{0.04}Sr_{0.01}K_{0.01})_{\Sigma 1.09}Al_{1.94}[(OH)_{1.92}(H_2O)_{0.08}]_{\Sigma 2.00}(V_{10}O_{28})$ •$27H_2O$. The simplified (ideal) structural formula of postite is $Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})$•$13H_2O$.

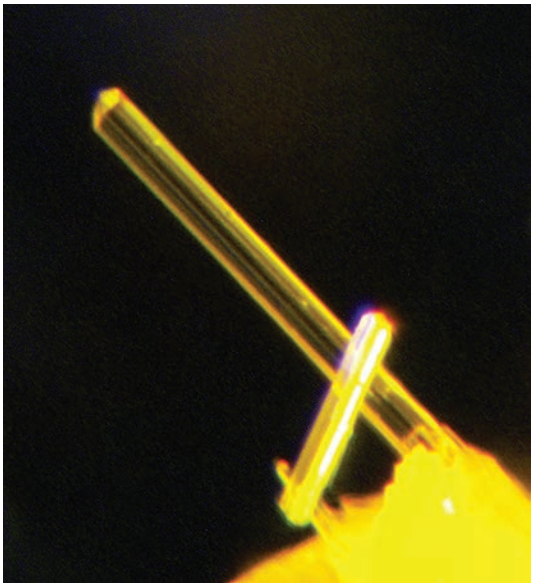

FIG 2. Individual crystal of postite from the Blue Cap mine (field of view is 2 mm).

The crystal structure determination (see below) provides the ideal formula $MgAl_2(OH)_2(V_{10}O_{28})\bullet 27H_2O$, with the structural formula written as $Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})\bullet 13H_2O$. Column 4 of Table 1 provides the normalized analytical results corresponding to the fully hydrated composition with 57 oxygen atoms, which yields the empirical formula $(Mg_{0.97}Na_{0.06}Ca_{0.04}Sr_{0.01}K_{0.01})_{\Sigma 1.09}Al_{1.94}[(OH)_2(H_2O)_{0.08}](V_{10}O_{28})\bullet 27H_2O$.

CRYSTAL STRUCTURE: EXPERIMENTAL

Powder and single-crystal X-ray diffraction data were obtained with a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer using monochromatized Mo*K*α radiation. The powder data presented in Table 2 are in good agreement with those calculated from the structure data. Observed *d* values and intensities were derived by profile fitting using JADE v. 9.3 software.

The Rigaku CrystalClear software package was used for processing of the structure data. The structure was solved by direct methods using SIR92 (Altomare *et al.* 1994). Because the crystals diffract weakly and occur as very thin needles, it was only possible to collect data to $2\theta_{max}$ = 41.64°. The SHELXL-97 software

TABLE 2. POWDER X-RAY DATA FOR POSTITE

I_{obs}	d_{obs}(Å)	d_{calc}(Å)	I_{calc}	*h k l*	I_{obs}	d_{obs}(Å)	d_{calc}(Å)	I_{calc}	*h k l*
90	12.190	12.1217	100	0 2 0	9	2.5911	2.5824	9	5 4 2
100	8.937	8.8696	89	1 1 1	10	2.4387	2.4408	3	4 5 3
22	8.248	8.1678	24	2 0 0			2.3702	3	1 8 3
8	7.245	7.2433	12	1 3 0	11	2.3354	2.3450	2	2 9 2
14	6.801	6.7736	15	2 2 0			2.3314	4	5 6 2
12	5.904	5.8672	11	0 0 2			2.2027	1	5 7 2
5	5.329	5.3129	2	3 1 0	3	2.2042	2.1983	1	1 9 3
		5.2811	3	0 2 2			2.1928	1	3 8 3
3	5.026	5.0250	2	1 2 2			2.1078	2	0 8 4
3	4.818	4.8672	3	2 4 0	8	2.1044	2.1073	2	5 3 4
		4.7478	2	0 3 2			2.0966	2	6 4 3
5	4.610	4.5742	2	3 2 1			2.0537	4	5 4 4
6	4.321	4.3215	4	1 5 1	13	2.0448	2.0444	3	1 10 3
24	3.771	3.7579	14	1 1 3			2.0409	2	2 8 4
6	3.482	3.4809	6	4 3 1			2.0294	5	6 5 3
13	3.335	3.3334	4	3 4 2	17	1.9907	1.9904	5	5 5 4
		3.3203	3	4 1 2			1.9841	2	0 9 4
		3.2608	4	1 6 2			1.9795	2	7 5 2
8	3.258	3.2551	3	1 7 1			1.9555	3	6 6 3
		3.2540	7	4 4 1			1.9319	1	5 8 3
19	2.9831	2.9825	7	0 7 2	4	1.9195	1.9281	1	2 9 4
		2.9336	3	0 0 4			1.9205	2	5 6 4
8	2.8447	2.8513	3	0 2 4			1.6196	2	5 13 0
		2.8395	2	3 6 2	4	1.6190	1.6189	1	10 2 0
4	2.7044	2.7094	3	5 5 0			1.6172	2	5 4 6

Note: Only calculated reflections with intensities greater than 2 are listed unless they correspond to observed lines.

(Sheldrick 2008) was used for the structure refinement, employing neutral-atom scattering factors. Hydrogen atoms were located using difference maps. Details of the crystal data, data collection, and structure refinement are provided in Table 3. Table 4 lists the atomic coordinates and equivalent displacement parameters, and Table 5 (on deposit) lists the anisotropic displacement parameters. Selected interatomic distances and bond valences are listed in Table 6. Hydrogen bonds linking the structural unit and the interstitial unit are listed in Table 7. A copy of Table 5, a table of structure factors and a CIF file are available from the Depository of Unpublished Data on the MAC website [document Postite CM50_45].

TABLE 3. CRYSTAL DATA, DATA COLLECTION, AND STRUCTURE REFINEMENT DETAILS FOR POSTITE

Chemical formula	$Mg(H_2O)_6Al_2(OH)_2(H_2O)_8(V_{10}O_{28})\bullet 13H_2O$
Formula weight	1556.12
Temperature	293(2) K
Wavelength	0.71075 Å
Crystal size	0.01 × 0.01 × 0.16 mm
Crystal system	Orthorhombic
Space group	*P c c n*
Unit cell dimensions	*a* = 16.3357(6) Å
	b = 24.2434(17) Å
	c = 11.7343(4) Å
Volume	4647 2(4) Å^3
Z	4
Density (calculated)	2.224 gm/cm^3
Absorption coefficient	2.110 mm^{-1}
F(000)	3120
Theta range for data collection	3.01 to 20.82°
Index ranges	$-16 \le h \le 16$, $-24 \le k \le 24$, $-11 \le l \le 11$
Reflections collected	29655
Independent reflections	2425 [*R*(int) = 0.1337]
Max. and min. transmission	0.9731 and 0.7289
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick 2008)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2425 / 35 / 429
Goodness-of-fit on F^2	1.004
Δ/Σ_{max}	0.001
Final *R* indices	
1583 data; $I > 2\Sigma(I)$	R_1 = 0.0358, wR_2 = 0.0668
all data	R_1 = 0.0739, wR_2 = 0.0775
Weighting scheme	$w = 1 / [\Sigma^2(F_o^2) + (0.0336P)^2 + 0.0000P]$ where $P = (F_o^2 + 2F_c^2) / 3$
Extinction coefficient	0.0003(1)
Largest diff. peak and hole	0.351 and –0.375 eÅ^{-3}

TABLE 4. COORDINATES AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS§ (Å^2) OF ATOMS IN POSTITE

	x/a	y/b	z/c	*U*(eq)
V1	0.94897(7)	0.01624(5)	0.38422(9)	0.0164(3)
V2	0.05671(6)	0.90690(5)	0.39871(10)	0.0185(3)
V3	0.04065(7)	0.12796(5)	0.38343(9)	0.0219(3)
V4	0.14300(6)	0.01971(5)	0.38876(9)	0.0176(3)
V5	0.86511(7)	0.90308(5)	0.39945(10)	0.0198(3)
Al1	0.94127(11)	0.95683(8)	0.00276(17)	0.0185(5)
Mg1	1/4	3/4	0.5738(3)	0.0501(12)
O1	0.0453(2)	0.98160(17)	0.3234(3)	0.0174(11)
O2	0.8775(2)	0.04320(16)	0.5025(3)	0.0174(11)
O3	0.9634(2)	0.88471(17)	0.3226(3)	0.0189(11)
O4	0.8794(2)	0.97699(17)	0.3158(4)	0.0186(11)
O5	0.9565(2)	0.07607(17)	0.3097(3)	0.0193(11)
O6	0.8830(2)	0.85095(17)	0.5109(3)	0.0207(11)
O7	0.1167(2)	0.08201(17)	0.3110(3)	0.0195(12)
O8	0.0465(2)	0.85751(16)	0.5145(4)	0.0207(11)
O9	0.2003(2)	0.05520(18)	0.5008(4)	0.0199(11)
O10	0.1288(3)	0.88076(18)	0.3228(4)	0.0263(13)
O11	0.7968(2)	0.87487(19)	0.3212(4)	0.0259(13)
O12	0.0347(3)	0.17922(17)	0.2964(4)	0.0310(12)
O13	0.2118(2)	0.99209(18)	0.3099(4)	0.0230(12)
O14	0.9618(2)	0.95102(17)	0.5029(3)	0.0169(10)
OH1	0.0264(3)	0.98487(18)	0.0892(3)	0.0192(11)
HOH	0.035(4)	0.985(3)	0.163(3)	0.05
OW1	0.9164(3)	0.9008(2)	0.1074(4)	0.0251(12)
H1a	0.874(3)	0.879(2)	0.100(5)	0.05
H1b	0.939(4)	0.896(3)	0.176(3)	0.05
OW2	0.8527(3)	0.9333(2)	0.9105(4)	0.0280(13)
H2a	0.857(4)	0.924(3)	0.838(3)	0.05
H2b	0.801(2)	0.940(3)	0.931(5)	0.05
OW3	0.9911(3)	0.09408(19)	0.0781(4)	0.0256(12)
H3a	0.996(4)	0.1290(15)	0.053(5)	0.05
H3b	0.971(4)	0.095(2)	0.149(3)	0.05
OW4	0.8627(3)	0.0055(2)	0.0757(4)	0.0267(13)
H4a	0.840(4)	0.006(3)	0.144(3)	0.05
H4b	0.842(4)	0.031(2)	0.033(4)	0.05
OW5a	0.1788(15)	0.7862(9)	0.4732(17)	0.052(6)
OW5b	0.1686(15)	0.7667(8)	0.4297(16)	0.046(5)
H5a	0.153(7)	0.749(4)	0.413(9)	0.05
H5b	0.152(6)	0.798(4)	0.483(9)	0.05
OW6a	0.3208(8)	0.7541(5)	0.7184(11)	0.052(4)
OW6b	0.3350(6)	0.6929(6)	0.6590(11)	0.050(4)
H6a	0.374(5)	0.690(4)	0.655(8)	0.05
H6b	0.324(5)	0.725(3)	0.728(8)	0.05
OW7a	0.1838(7)	0.6881(5)	0.6177(14)	0.049(4)
OW7b	0.1914(8)	0.6722(5)	0.5237(12)	0.050(4)
H7a	0.187(5)	0.649(3)	0.562(7)	0.05
H7b	0.147(5)	0.688(3)	0.638(7)	0.05
OW8	0.7945(3)	0.8291(2)	0.0775(4)	0.0365(14)
H8a	0.742(2)	0.836(3)	0.071(6)	0.05
H8b	0.808(4)	0.803(2)	0.028(5)	0.05
OW9	0.0171(3)	0.7994(2)	0.9644(4)	0.0452(15)
H9a	–0.028(3)	0.784(3)	0.939(5)	0.05
H9b	0.024(4)	0.796(3)	1.038(3)	0.05
OW10	0.0216(3)	0.7889(2)	0.2046(4)	0.0428(15)
H10a	–0.001(4)	0.7566(15)	0.212(6)	0.05
H10b	0.006(4)	0.8148(18)	0.250(5)	0.05
OW11	0.7240(3)	0.0683(2)	0.4147(5)	0.0440(15)
H11a	0.773(3)	0.058(3)	0.442(5)	0.05
H11b	0.716(4)	0.051(3)	0.349(4)	0.05
OW12	0.8137(5)	0.1329(3)	0.1805(11)	0.133(4)
H12a	0.837(4)	0.158(3)	0.219(7)	0.05
H12b	0.770(3)	0.142(3)	0.143(6)	0.05
OW13	0.8623(4)	0.7436(2)	0.4225(5)	0.0478(16)
H13a	0.870(4)	0.7757(17)	0.452(5)	0.05
H13b	0.838(4)	0.742(3)	0.359(4)	0.05
OW14	3/4	3/4	0.2480(7)	0.045(2)
H14	0.733(4)	0.719(2)	0.214(6)	0.05

§*U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

TABLE 6. SELECTED BOND DISTANCES (Å) AND BOND-VALENCE VALUES (*vu*) IN POSTITE

V1–	Distance	Valence	V2–	Distance	Valence
O4	1.685(4)	1.38	O10	1.607(4)	1.70
O5	1.698(4)	1.33	O8	1.819(4)	0.96
O1	1.921(4)	0.73	O3	1.847(4)	0.89
O2	1.928(4)	0.71	O2	1.991(4)	0.60
O14	2.117(4)	0.43	O1	2.024(4)	0.55
O14'	2.123(4)	0.42	O14	2.245(4)	0.30
Mean, Sum:	1.912	5.00	Mean, Sum:	1.922	5.00
V3–	Distance	Valence	V4–	Distance	Valence
O12	1.611(4)	1.68	O13	1.602(4)	1.72
O6	1.832(4)	0.92	O7	1.816(4)	0.97
O7	1.873(4)	0.83	O9	1.828(4)	0.93
O8	1.893(4)	0.78	O1	1.998(4)	0.59
O5	2.054(4)	0.51	O2	2.016(4)	0.56
O14	2.334(4)	0.24	O14	2.248(4)	0.30
Mean, Sum:	1.933	4.96	Mean, Sum:	1.918	5.07
V5–	Distance	Valence	Mg–	Distance	Valence
O11	1.599(4)	1.74	OW5a	1.88(2)	0.60
O6	1.842(4)	0.90	OW7a	1.920(11)	0.54
O9	1.880(4)	0.81	OW6a	2.056(14)	0.37
O3	1.894(4)	0.78	OW5b	2.189(19)	0.26
O4	2.056(4)	0.50	OW7b	2.196(13)	0.26
O14	2.306 (4)	0.26	OW6b	2.201(13)	0.25
Mean, Sum:	1.930	4.99	Mean, Sum:	2.074	2.28
Al–	Distance	Valence			
OH1	1.851(5)	0.58			
OH1'	1.855(5)	0.58			
OW1	1.876(5)	0.54			
OW2	1.895(5)	0.52			
OW3	1.909(5)	0.50			
OW4	1.943(5)	0.45			
Mean, Sum:	1.888	3.17			

Bond Sums for Oxygen Atoms*

O1:	1.87(1.95)	O2:	1 87(1.95)	O3:	1.67(1.77)	O4:	1.88(1.88)
O5:	1.84(1.91)	O6:	1 82(1.92)	O7:	1.80(1.90)	O8:	1.74(1.74)
O9:	1.74(1.81)	O10:	1.70(1.70)	O11:	1.74(1.74)	O12:	1.68(1.75)
O13:	1.72(1.80)	O14:	1 95(1.95)				

Bond Sums for Hydroxyl, H_2O Molecules

OH1:	1.16	OW1:	0.54	OW2:	0.52	OW3:	0.50	OW4:	0.45	OW5a:	0.60
OW5b:	0 26	OW6a:	0.37	OW6b:	0.25	OW7a:	0.54	OW7b:	0 26		

OW8 through OW14 exist as isolated H_2O molecules.

*For oxygen atoms of the decavanadate polyanion, bond sums in parentheses include the bond valence for the hydrogen bonds listed in Table 7. Bond valences were calculated using the parameters in Brese & O'Keeffe (1991).

Atomic Arrangement of Postite

Minerals containing the decavanadate group can be considered members of the pascoite family, pascoite [$Ca_3(V_{10}O_{28})$•$17H_2O$] being the first described decavanadate mineral. All of the minerals of the pascoite family possess bipartite structures that contain a *structural unit* and an *interstitial unit*, as elucidated by Hawthorne (1983). The $[V_{10}O_{28}]^{6-}$ polyanion (assuming the unprotonated polyanion) defines the structural unit,

the anhydrous anionic portion of the structure. The structural units are linked by the interstitial unit, the cationic portion of the structure, with bonds of lower bond-valence linking alkalis, alkaline earths, aluminum, and OH and H_2O groups to oxygen atoms of the structural unit (Hughes *et al*. 2008). Minerals of the pascoite family differ in (1) the extent of protonation of the decavanadate polyanion, if any, and (2) the composition and structure of the interstitial unit, which balances the charge of the decavanadate polyanion. Figure 3 depicts the disposition of the structural unit and interstitial unit in postite.

The structural unit in postite

The structural unit in postite is the decavanadate polyanion, similar to that found in structurally related minerals (Fig. 4). The decavanadate polyanion consists of ten distorted, edge-sharing octahedra. In the V2, V3, V4, and V5 octahedra in postite, each octahedron contains one vanadyl bond, defined as a V^{5+}–O bond less than 1.74 Å in length (Schindler *et al*. 2000). The V1 octahedron has two vanadyl bonds. In all cases, vanadyl bonds are *trans* to the longest V–O bond(s) of the octahedron, typical of the disposition of bonds in the octahedra of the decavanadate polyanion.

Recently, decavanadate minerals (rakovanite, gunterite) have been discovered that contain protonated decavanadate groups (see Duraisamy *et al*. 2000 for a summary of the protonated decavanadate polyanion). In postite, the decavanadate polyanion is not protonated, and the only non-protonated oxygen atoms occur within the decavanadate polyanion.

The interstitial unit in postite and its linkage with the structural unit

To balance the residual 6– charge of the decavanadate polyanion, the interstitial unit in postite of composition $[Mg(H_2O)_6Al_2(OH)_2(H_2O)_8 \bullet 13H_2O]^{6+}$ provides the cationic charge. The interstitial unit consists of a $[Mg(H_2O)_6]^{2+}$ monomer, an $[Al_2(OH)_2(H_2O)_8]^{4+}$ edge-sharing dimer, and thirteen additional H_2O molecules (OW8–OW14) (Fig. 3).

Notably, all the oxygen atoms in the interstitial unit are protonated, either as a hydroxyl or H_2O molecule, and no cations of the interstitial unit bond to oxygen atoms of the decavanadate structural unit; the linkage between the structural unit and the interstitial unit results entirely from hydrogen bonding. Table 7 lists the hydrogen bonds between the oxygen atoms of the structural unit and hydrogen atoms, which correspond to H–O distances less than 2.2 Å. The decavanadate polyanion is linked to the $[Mg(H_2O)_6Al_2(OH)_2(H_2O)_8 \bullet 13 H_2O]^{6+}$ interstitial unit only through hydrogen bonding to hydrogen atoms associated with the oxygen atoms of the $[Al_2(OH)_2(H_2O)_8]^{4+}$ edge-sharing dimer (HOH, H3b, H2a, H2b, and H4a) and to those hydrogen atoms associated with isolated H_2O molecules (H11a, H11b, H8a, H13a, H10a, and H11b). The $[Mg(H_2O)_6]^{2+}$ monomer is not linked to the decavanadate polyanion through sharing of oxygen atoms or hydrogen bonding.

Disorder in the interstitial unit

During solution and refinement of the postite atomic arrangement, it was evident that there is extensive disorder of several of the oxygen atoms of the interstitial unit. Although the data were limited to relatively low diffraction angles ($2\theta_{max}$ = 41.64°), we were able to successfully refine the disorder of those oxygen atoms associated with the Mg octahedron (OW5, OW6, and OW7; note that in Table 4 the hydrogen atom positions are for the pre-split single oxygen site, as the data did not support modeling of the half-occupied H positions). In addition, OW12, an isolated H_2O molecule of the interstitial unit, indicated disorder, but that was not modeled owing to the already-low observation to parameter ratio. The $[Mg(OH_2)_6]$ monomer exhibits orientational disorder, and the likely reason is that a single hydrogen-bonding arrangement does not have significant preference over another.

TABLE 7. HYDROGEN BONDS (O–H…O ≤ 2.20 Å) BETWEEN THE STRUCTURAL UNIT AND INTERSTITIAL UNIT IN POSTITE

Oxygen	Hydrogen	Distance*	Oxygen	Hydrogen	Distance
O1:	HOH	1.88	O2:	H11a	1.88
O3:	H1b	1.79	O5:	H3b	1.96
O6:	H8a	2.19	O6:	H13a	1.96
O7:	H2a	1.81	O9:	H2b	1.84
O12:	H10a	1.96	O13:	H4a	2.16
O13:	H11b	2.14			

*Distance in Å.

ACKNOWLEDGMENTS

The authors gratefully acknowledge Editor-in-Chief Robert F. Martin for his long-standing and insightful contributions to mineralogy through his service to *The Canadian Mineralogist*. The manuscript was improved by reviews by William S. Wise and an anonymous reviewer. This study was funded, in part, by the John Jago Trelawney Endowment to the Mineral Sciences Department of the Natural History Museum of Los Angeles County and by grant NSF-MRI 1039436 from the National Science Foundation to JMH.

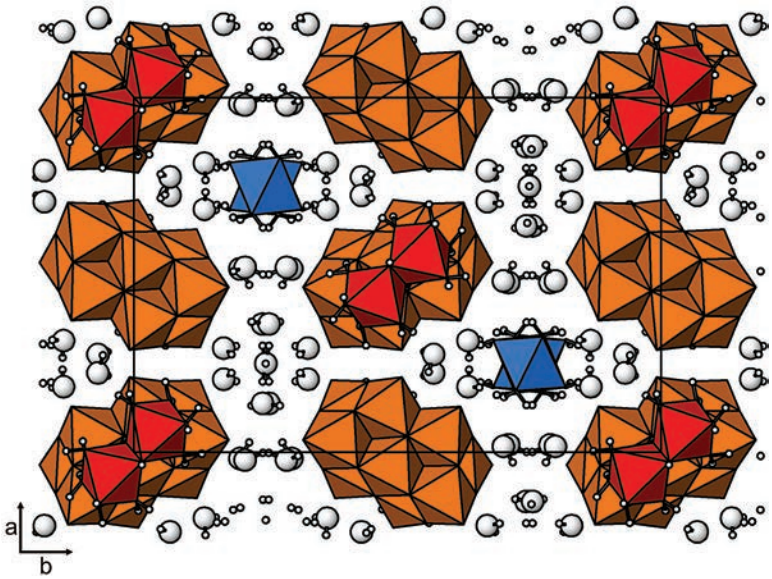

FIG 3. The atomic arrangement of postite. The decavanadate polyanion is depicted in brown and the $[Mg(H_2O)_6]^{2+}$ monomer is depicted in blue. The $[Al_2(OH)_2(H_2O)_8]^{4+}$ edge-sharing dimer is depicted in red. The disorder modeled for H_2O molecules OW5, OW6, and OW7 is not shown.

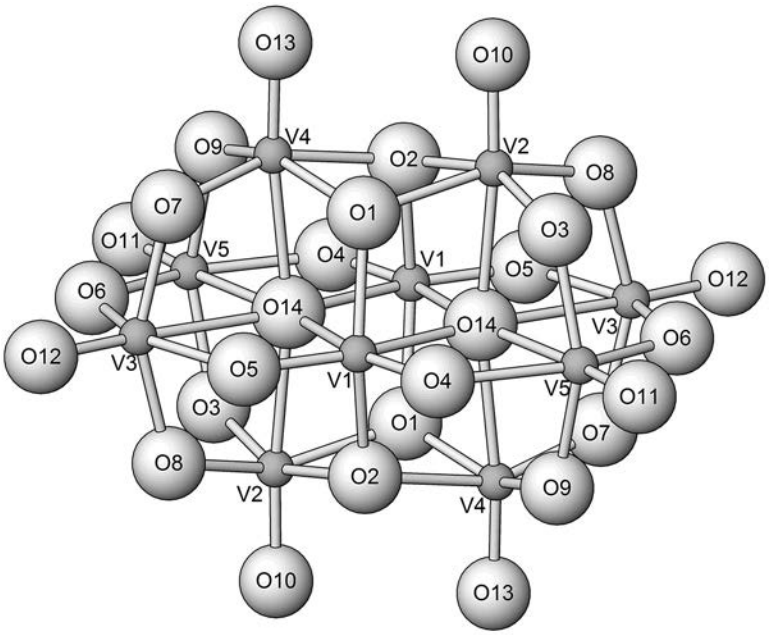

FIG 4. The decavanadate cluster in postite.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C., Polidori, G., & Camalli, M. (1994) SIR92 - a program for automatic solution of crystal structures by direct methods. *Journal of Applied Crystallography* **27,** 435.

Brese, N.E. & O'Keeffe, M. (1991) Bond-valence parameters for solids. *Acta Crystallographica* **B47**, 192-197.

Carter, W.D. & Gualtieri, J.L. (1965) Geology and uranium–vanadium deposits of the La Sal quadrangle, San Juan County, Utah, and Montrose County, Colorado. *United States Geological Survey, Professional Paper* **508**.

Colombo, F., Baggio, R., & Kampf, A.R. (2011) The crystal structure of the elusive huemulite. *Canadian Mineralogist* **49**, 849-864.

Duraisamy, T., Ramanan, A., & Vittal, J.J. (2000): Novel self-assembled decavanadate clusters forming 1D molecular chains and 2D molecular arrays: [HMTA-H$\cdots$ H_2O][HMTA-CH_2OH][$H_3V_{10}O_{28}${$NaH_2O)_4$}]•$4H_2O$ and [$Na_2(H_2O)_{10}$] [$H_3V_{10}O_{28}${$Na(H_2O)_2$}]•$3H_2O$. *Crystal Engineering* **3**, 237-250.

Evans, H.T., Jr., & Garrels, R.M. (1958) Vanadium in aqueous solution as applied to the interpretation of the Colorado Plateau ore deposits. *Geochimica Cosmochimica Acta* **15**, 131-149.

Gordillo, C.E., Linares, E., Toubes , R.O. & Winchell, H. (1966) Huemulite, $Na_4MgV_{10}O_{24}$•$24H_2O$, a new hydrous sodium and magnesium vanadate from Huemul mine, Mendoza Province, Argentina. *American Mineralogist* **51**, 1-13.

Hawthorne, F.C. (1983) Graphical enumeration of polyhedral clusters. *Acta Crystallographica* **A39**, 724-736.

Hughes, J.M., Cureton, F.E., Marty, J., Gault, R.A., Gunter, M.E., Campana, C.F., Rakovan, J., Sommer, A. & Brueseke, M.E. (2001) Dickthomssenite, $Mg(V_2O_6)$•$7H_2O$, a new mineral from the Firefly–Pigmay mine, Utah: descriptive mineralogy and arrangement of atoms. *Canadian Mineralogist* **39**, 1691-1700.

Hughes, J.M., Schindler, M., Rakovan, J. & Cureton, F.E. (2002) The crystal structure of hummerite, $KMg(V_5O_{14})$•$8H_2O$: bonding between the $[V_{10}O_{28}]^{6-}$ structural unit and the $\{K_2Mg_2(H_2O)_{16}\}^{6+}$ interstitial complex. *Canadian Mineralogist* **40**, 1429-1435.

Hughes, J.M., Schindler, M. & Francis, C.A. (2005) The *C2/m* disordered structure of pascoite, $Ca_3[V_{10}O_{28}]$•$17H_2O$: bonding between structural units and interstitial complexes in compounds containing the $[V_{10}O_{28}]^{6-}$ decavanadate polyanion. *Canadian Mineralogist* **43**, 1379-1386.

Hughes, J.M., Wise, W.S., Gunter, M.E., Morton, J.P., & Rakovan, J. (2008) Lasalite, $Na_2Mg_2[V_{10}O_{28}]$•$20H_2O$, a new decavanadate mineral species from the Vanadium Queen Mine, La Sal District, Utah: Description, atomic arrangement, and relationship to the pascoite group of minerals. *Canadian Mineralogist* **46**, 1365-1372.

Kampf, A.R. & Steele, I.M. (2008a) Magnesiopascoite, a new member of the pascoite group: description and crystal structure. *Canadian Mineralogist* **46**, 679-686.

Kampf, A.R. & Steele, I.M. (2008b) Martyite, a new mineral related to volborthite: Description and crystal structure. *Canadian Mineralogist* **46**, 687-692.

Kampf, A.R., Hughes, J.M., Marty, J., Gunter, M.E., & Nash, B. (2011a) Rakovanite, Na_3{$H_3[V_{10}O_{28}]$}•$15H_2O$, a new species of the pascoite family with a protonated decavanadate polyanion. *Canadian Mineralogist* **49**, 889-898.

Kampf, A.R., Hughes, J.M., Marty, J., & Nash, B. (2011b) Gunterite, $Na_4(H_2O)_{16}(H_2V_{10}O_{28})$•$6H_2O$, a new mineral with a doubly-protonated decavanadate polyanion: Crystal structure and descriptive mineralogy. *Canadian Mineralogist* **49**, 1243-1251.

Pouchou, J.-L. & Pichoir, F. (1991) Quantitative analysis of homogeneous or stratified microvolumes applying the model "PAP." *In* K.F.J. Heinrich & D.E. Newbury, Eds. Electron Probe Quantitation, p. 3l-75. Plenum Press, New York.

Rakovan, J., Schmidt, G.R., Gunter, M., Nash, B., Kampf, A.R., Marty, J., & Wise, W.S. (2011) Hughesite, $Na_3Al(V_{10}O_{28})$•$22H_2O$, a new member of the pascoite family of minerals from the Sunday mine, San Miguel County, Colorado. *Canadian Mineralogist* **49**, 1253-1265.

Schindler, M., Hawthorne, F.C., & Baur, W.H. (2000) Crystal-chemical aspects of vanadium: polyhedral geometries, characteristic bond valences, and polymerization of (VO_n) polyhedral. *Chemistry of Materials* **12**, 1248-1259.

Shawe, D.R. (2011) Uranium-vanadium deposits of the Slick Rock district, Colorado. *United States Geological Survey, Professional Paper* **576-F**, 80 p., 20 plates.

Sheldrick, G.M. (2008) A short history of *SHELX*. *Acta Crystallographica* **A64**, 112-122.

Received October 11, 2011, revised manuscript accepted January 30, 2012.